ANALYSIS OF NON-ORTHOGONAL n-WAY CLASSIFICATIONS AND FRACTIONAL REPLICATION

BU-254-M

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Abstract

A calculus of the factorials was developed by Kurkjian and Zelen in 1962 and two papers on applications and extensions to unequal numbers analyses for n-way classifications were presented by Zelen and Federer. Some of the remaining problems associated with the application of the calculus of factorials is to obtain expected values of the sums of squares for fixed, mixed, and random models, and to obtain analyses for single degree of freedom or sets of degree of freedom contrasts and their expectations under the various models. These problems were resolved in the present paper, and are presented in rather simple forms.

It is known that a sum of squares in the analysis of variance is invariant under linear transformation and this suggests that some appropriate linear transformation will be useful in using the calculus of factorials. Our calculation is based on this principle, i.e., we use the class means in a multiple classification and apply the orthogonal transformation to the parameters using orthogonal contrasts of levels of factors. A numerical example is used to illustrate the procedure.

After slight modification, a Kronecker product representation is given for the design matrix of an n-factor-factorial and a method of constructing fractional replicates is developed. Special reference is made to the construction of saturated main effect fractional replicates, and an invariant property of the information matrix is investigated. Finally, a randomized procedure which is similar to Ehrenfeld and Zacks R.P.I. is developed for non-orthogonal saturated main effect fractional replicates.

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1. Introduction

The calculus of factorials was introduced by Kurkjian and Zelen [1962] and was extended and applied by Kurkjian and Zelen [1963] and Zelen and Federer [1964,1965,1966]. The last two papers dealt with unequal numbers analysis. Three of the remaining problems associated with these analyses were (i) to obtain analyses when some of the effect parameters are zero (Paik and Federer [1967b]), (ii) to obtain analyses when some of the subclasses are empty, and (iii) to obtain expected values for the sums of squares in the analysis of variance for fixed, mixed, and random models with or without missing subclasses. These problems have been resolved in the present study.

Another seemingly unrelated set of problems has to do with construction, optimality properties, and estimation of fractional replicates from any factorial. When there are missing subclasses in an n-way classification a fractional replicate results. A general procedure has been developed (Paik and Federer [1967b]) for constructing saturated fractional replicates for <u>any</u> specified set of treatment parameters. Since there are often numerous plans for any specified set of parameters, the question of which set is best for the criteria considered arises. An investigation was carried out to determine the optimum saturated main effect plans for 2^2, 2^3, 2^4, 3^2, and 3^3 factorials, using the criterion that the determinant of the covariance matrix be a minimum. A randomized procedure is discussed for obtaining fractional replicates yielding unbiased estimators of the main effect parameters.

2. Notation

In a one-way classification let the j^{th} observation on the i^{th} treatment be represented as:

$$y_{ij} = \mu_i + \epsilon_{ij} = \mu + \alpha_i + \epsilon_{ij}$$

where $i=0,1,2,\cdots,t-1$; $j=1,2,\cdots,r_i$; μ is an unknown parameter common to every observation, α_i is an unknown parameter related to the i^{th} treatment, and we assume that

$$E\epsilon_{ij} = 0$$

$$\operatorname{cov}(\epsilon_{ij}\epsilon_{i'j'}) = \begin{cases} \sigma_\epsilon^2 & \text{for } ij = i'j' \\ 0 & \text{for } ij \neq i'j' \end{cases} .$$

Instead of utilizing the α_i parameters let us transform the $\{\alpha_i;\ i=0,1,\cdots,t-1\}$ into another set of constants $\{a_m;\ m=0,1,\cdots,t-1\}$ by utilizing a set of orthogonal contrasts (e.g., orthogonal polynomials) among the t constants as follows:

$$\alpha_i = \sum_{m=0}^{t-1} a_m p_m(i)$$

where the $p_m(i)$ are functions of powers of $(i-\bar{i})$ equal to or less than m such that

$$p_0(i) = 1/\sqrt{t} \quad \text{for all } i$$

$$\sum_{i=0}^{t-1} p_m(i)p_{m'}(i) = \begin{cases} 1 & \text{if } m = m' \\ 0 & \text{if } m \neq m' \end{cases} .$$

In matrix notation the above becomes

$$\underline{\alpha} = P\underline{a}$$

where $\underline{\alpha}' = (\alpha_0,\alpha_1,\cdots,\alpha_{t-1})$, $\underline{a}' = (a_0,a_1,\cdots,a_{t-1})$, and P is a t x t matrix of the following form:

$$\begin{bmatrix} 1/\sqrt{t} & p_1(0) & p_2(0) & \cdots & p_{t-1}(0) \\ 1/\sqrt{t} & p_1(1) & p_2(1) & \cdots & p_{t-1}(1) \\ 1/\sqrt{t} & p_1(2) & p_2(2) & \cdots & p_{t-1}(2) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1/\sqrt{t} & p_1(t-1) & p_2(t-1) & \cdots & p_{t-1}(t-1) \end{bmatrix}$$

Then $P'P = I_{txt}$ and $\underline{a} = P'\underline{\alpha}$. This implies that if $a_1=a_2=\cdots=a_{t-1}=0$ then $\alpha_0=\alpha_1=\alpha_2=\cdots=\alpha_{t-1}$. Now, if $E\underline{\alpha\alpha}' = I\sigma_\alpha^2$, then $E\underline{aa}' = I\sigma_\alpha^2$.

In a two-way classification the k^{th} observation on the ij^{th} combination of two factors with interaction may be denoted by

$$y_{ijk} = \mu_{ij} + \epsilon_{ijk} = \mu + \alpha_i + \beta_j + \alpha\beta_{ij} + \epsilon_{ijk} \qquad (2.1)$$

where $k=1,2,\cdots,r_{ij}\geq 1$; $i\overset{0}{=}1,2,\cdots,t-1$; $j\overset{0}{=}1,2,\cdots,u-1$; μ is an unknown parameter common to every observation, the $\{\alpha_i\}$ is a set of unknown parameters related to one factor, the $\{\beta_j\}$ is a set of unknown parameters related to a second factor, and the $\{\alpha\beta_{ij}\}$ is a set of unknown interaction parameters related to a specific combination of levels of the two factors. We assume that

$$E\epsilon_{ijk} = 0$$

$$\mathrm{cov}(\epsilon_{ijk}\epsilon_{i'j'k'}) = \begin{cases} \sigma_\epsilon^2 & \text{for } ijk = i'j'k' \\ 0 & \text{for } ijk \neq i'j'k' \end{cases} .$$

As in the one-way classification we shall use a transformation of the α_i, β_j, and $\alpha\beta_{ij}$ parameters as follows:

$$\alpha_i = \sum_{m=0}^{t-1} a_m p_m(i)$$

$$\beta_j = \sum_{n=0}^{u-1} b_n q_n(j)$$

$$\alpha\beta_{ij} = \sum_{m=0}^{t-1} \sum_{n=0}^{u-1} c_{mn} p_m(i) q_n(j) \tag{2.2}$$

where a_m, b_n, and c_{mn} are unknown parameters and $p_m(i)$ and $q_n(j)$ are functions of powers of $(i-\bar{i})$ less than or equal to m and powers of $(j-\bar{j})$ less than or equal to n, respectively, such that

$$p_0(i) = 1/\sqrt{t} \quad \text{for all } i ,$$

$$q_0(j) = 1/\sqrt{u} \quad \text{for all } j ,$$

$$\sum_{i=0}^{t-1} p_m(i) p_{m'}(i) = \begin{cases} 1 & \text{if } m = m' \\ 0 & \text{if } m \neq m' \end{cases} ,$$

and

$$\sum_{j=1}^{u-1} q_n(j)q_{n'}(j) = \begin{cases} 1 & \text{if } n = n' \\ 0 & \text{if } n \neq n' \end{cases} . \tag{2.3}$$

Given that $\mu_{ij} = \mu + \alpha_i + \beta_j + \alpha\beta_{ij}$ we rewrite the foregoing as:

$$\mu_{ij} = \mu^+ + \sum_{m=1}^{t-1} a_m^+ p_m(i) + \sum_{n=1}^{u-1} b_n^+ q_n(j) + \sum_{m=1}^{t-1}\sum_{n=1}^{u-1} c_{mn}p_m(i)q_n(j)$$

where

$$\mu^+ = \mu + a_0p_0(i) + b_0q_0(j) + c_{00}p_0(i)q_0(j) \quad ,$$

$$a_m^+ = a_m + c_{m,0}q_0(j) \quad ,$$

and

$$b_n^+ = b_n + c_{0,n}p_0(i) \quad . \tag{2.4}$$

Using vector or matrix notation, we define

$\underline{y} = (y_{001}, y_{002}, \cdots, y_{t-1,u-1,r_{t-1,u-1}})'$

$\underline{1}_N$ = N x 1 column vector with all elements equal to one

$\underline{\epsilon} = (\epsilon_{001}, \epsilon_{002}, \cdots, \epsilon_{t-1,u-1,r_{t-1,u-1}})'$

$\underline{\mu} = (\mu_{00}, \mu_{01}, \cdots, \mu_{t-1,u-1})'$

$\underline{\alpha} = (\alpha_0, \alpha_1, \cdots, \alpha_{t-1})'$

$$\underline{\beta} = (\beta_0, \beta_1, \cdots, \beta_{u-1})'$$

$$\underline{\alpha\beta} = (\alpha\beta_{00}, \alpha\beta_{01}, \cdots, \alpha\beta_{t-1,u-1})'$$

$$\underline{a}^* = (a_0, a_1, \cdots, a_{t-1})'$$

$$\underline{b}^* = (b_0, b_1, \cdots, b_{u-1})'$$

$$\underline{c}^* = (c_{00}, c_{01}, \cdots, c_{t-1,u-1})'$$

$$\underline{c}_{m\cdot} = (c_{10}, c_{20}, \cdots, c_{t-1,0})'$$

$$\underline{c}_{\cdot n} = (c_{01}, c_{02}, \cdots, c_{0,u-1})'$$

$$\underline{a} = (a_1, a_2, \cdots, a_{t-1})'$$

$$\underline{b} = (b_1, b_2, \cdots, b_{u-1})'$$

$$\underline{a}^+ = (a_1^+, a_2^+, \cdots, a_{t-1}^+)'$$

$$\underline{b}^+ = (b_1^+, b_2^+, \cdots, b_{u-1}^+)'$$

$$\underline{c} = (c_{11}, c_{12}, \cdots, c_{t-1,u-1})'$$

$$\underline{p}_m = (p_m(0), p_m(1), \cdots, p_m(t-1))'$$

$$\underline{q}_n = (q_n(0), q_n(1), \cdots, q_n(u-1))'$$

$$\underline{w}_{mn} = (p_m(0)q_n(0), p_m(0)q_n(1), \cdots, p_m(t-1)q_n(u-1))'$$

$$p^* = (\underline{p}_0, \underline{p}_1, \cdots, \underline{p}_{t-1}) \text{ , i.e., } p^* \text{ is a } t \times t \text{ matrix}$$

$$q^* = (\underline{q}_0, \underline{q}_1, \cdots, \underline{q}_{u-1}) \text{ , i.e., } q^* \text{ is a } u \times u \text{ matrix}$$

$$W^* = (\underline{w}_{00}, \underline{w}_{01}, \cdots, \underline{w}_{t-1,u-1}) \text{ , i.e., } W^* \text{ is a } tu \times tu \text{ matrix}$$

$$p = (\underline{p}_1, \underline{p}_2, \cdots, \underline{p}_{t-1}) \text{ , i.e., } p \text{ is a } t \times (t-1) \text{ matrix}$$

$$q = (\underline{q}_1, \underline{q}_2, \cdots, \underline{q}_{u-1}) \text{ , i.e., } q \text{ is a } u \times (u-1) \text{ matrix}$$

$$W_m = (\underline{w}_{10}, \underline{w}_{20}, \cdots, \underline{w}_{t-1,0}) \text{ , i.e., } W_m \text{ is a } tu \times (t-1) \text{ matrix}$$

$$W_n = (\underline{w}_{01}, \underline{w}_{02}, \cdots, \underline{w}_{0,u-1}) \text{ , i.e., } W_n \text{ is a } tu \times (u-1) \text{ matrix}$$

$$W = (\underline{w}_{11}, \underline{w}_{12}, \cdots, \underline{w}_{t-1,u-1}) \text{ , i.e., } W \text{ is a } tu \times (t-1)(u-1) \text{ matrix}$$

Then (2.1) and (2.2) may be represented as follows:

$$\underline{y} = X\underline{\mu} + \underline{\epsilon} \tag{2.5}$$

$$\underline{\alpha} = p^*\underline{a}^* \text{ ,}$$

$$\underline{\beta} = q^*\underline{b}^* \text{ ,}$$

and

$$\underline{\alpha\beta} = W^*\underline{c}^* \text{ ,} \tag{2.6}$$

where X is an N $\times$ tu design matrix with respect to parameter $\underline{\mu}$.

Let P* and Q* be tu $\times$ t and tu $\times$ u matrices, respectively, and satisfy the following equation

$$\underline{\mu} = \mu \underline{1}_{tu} + P^* \underline{a}^* + Q^* \underline{b}^* + W^* \underline{c}^* \quad ; \tag{2.7}$$

let P and Q be the tu × (t-1) and tu × (u-1) matrices, respectively; and let P_m and Q_n be the tu × 1 column vectors such that

$$P^* = \left[\frac{1}{\sqrt{t}} \underline{1}_{tu} P \right] = \left[\frac{1}{\sqrt{t}} \underline{1}_{tu}, P_1, P_2, \cdots, P_{t-1} \right]$$

and

$$Q^* = \left[\frac{1}{\sqrt{u}} \underline{1}_{tu} Q \right] = \left[\frac{1}{\sqrt{u}} \underline{1}_{tu}, Q_1, Q_2, \cdots, Q_{u-1} \right] .$$

Then,

$$P^{*\prime} P^* = uI_{t\times t} , \quad P'P = uI_{(t-1)\times(t-1)} , \quad P_m' P_m = u$$

$$Q^{*\prime} Q^* = tI_{u\times u} , \quad Q'Q = tI_{(u-1)\times(u-1)} , \text{ and } Q_n' Q_n = t \quad .$$

Equation (2.7) can then be represented as follows:

$$\underline{\mu} = \mu^+ \underline{1}_{tu} + P\underline{a}^+ + Q\underline{b}^+ + W\underline{c} \quad . \tag{2.8}$$

The least-squares solution of (2.5) is

$$\hat{\mu} = S^{-1} X' \underline{y} \tag{2.9}$$

where $S^{-1} = (X'X)^{-1}$.

From (2.8)

$$\mu^+ = \frac{1}{tu} \underline{1}_{tu}\underline{\mu} \quad ,$$

$$\underline{a}^+ = \frac{1}{u} P'\underline{\mu} \quad ,$$

$$\underline{b}^+ = \frac{1}{t} Q'\underline{\mu} \quad ,$$

and

$$\underline{c} = W'\underline{\mu} \quad . \tag{2.10}$$

Then,

$$\hat{\underline{a}}^+ = \frac{1}{u} P'\hat{\underline{\mu}} \quad ,$$

$$\hat{\underline{b}}^+ = \frac{1}{t} Q'\hat{\underline{\mu}} \quad ,$$

and

$$\hat{\underline{c}} = W'\hat{\underline{\mu}} \quad . \tag{2.11}$$

From (2.6), we note that

$$a_1 = a_2 = \cdots = a_{t-1} = 0 \text{ implies } \alpha_0 = \alpha_1 = \cdots = \alpha_{t-1}$$

$$b_1 = b_2 = \cdots = b_{u-1} = 0 \text{ implies } \beta_0 = \beta_1 = \cdots = \beta_{u-1}$$

and

$$c_{01} = c_{02} = \cdots = c_{t-1,u-1} = 0 \text{ implies}$$

$$\alpha\beta_{00} = \alpha\beta_{01} = \cdots = \alpha\beta_{t-1,u-1} \quad .$$

If

$$\text{Cov}(\underline{\alpha}) = I_{t\times t}\sigma^2_\alpha \quad ,$$

$$\text{Cov}(\underline{\beta}) = I_{u\times u}\sigma^2_\beta \quad ,$$

and

$$\text{Cov}(\underline{\alpha\beta}) = I_{tu \times tu}\sigma^2_{\alpha\beta} \quad ,$$

then

$$E\ a_m^2 = \sigma^2_\alpha \quad \text{for} \quad m=1,2,\cdots,t-1 \quad ,$$

$$E\ b_n^2 = \sigma^2_\beta \quad \text{for} \quad n=1,2,\cdots,u-1 \quad ,$$

and

$$E\ c_{mn}^2 = \sigma^2_{\alpha\beta} \quad \text{for } mn = 01;02;\cdots;t-1,u-1 \quad .$$

The extension of the above notation to the general n-way classification is straightforward in that it follows directly from the material given above, i.e., the main effects and interaction parameter vectors corresponding to $\underline{a}^*$, $\underline{b}^*$, and $\underline{c}^*$ in two-way classification may be defined as

$$\underline{a}_1^* = (a_1(0), a_1(1), \cdots, a_1(t_1-1))'$$

$$\underline{a}_2^* = (a_2(0), a_2(1), \cdots, a_2(t_2-1))' \quad .$$

and

$$\underline{a}_{12}^* = (a_{12}(0,0), a_{12}(0,1), \cdots, a_{12}(t_1-1, t_2-1))'$$

and matrices corresponding to p^*, q^*, and W^* may be defined as p_1^*, p_2^*, and W_{12}^*. From this, the extension to $3,4,\cdots,n$ factors is obvious.

3. Expectation of Mean Squares (in Anovas) ($r_{ij} \geq 1$)

We shall obtain the expected value of the sums of squares in the analysis of variance for the fixed, mixed, and random effects models for the two-way classification with unequal numbers of observations, $r_{ij} \geq 1$, in the subclasses. Extension to n-way classifications is straightforward. The sums of squares used in the analysis of variance are those given by Yates [1934] for the two-way classification and by Zelen and Federer [1965,1966] for the n-way classification.

The within subclasses sum of squares is given by:

$$\begin{aligned} SS_e &= \sum_{i=0}^{t-1} \sum_{j=0}^{u-1} \sum_{k=1}^{r_{ij}} (y_{ijk}-\bar{y}_{ij.})^2 \\ &= (\underline{y}-X\hat{\underline{\mu}})'(\underline{y}-X\hat{\underline{\mu}}) = \underline{y}'\underline{y} - y'XS^{-1}X'y \\ &= \underline{y}'(I-XS^{-1}X')\underline{y} \quad , \end{aligned} \tag{3.1}$$

where $S^{-1} = (X'X)^{-1}$. The expected value of SS_e, which has (N-tu) degrees of freedom, is $(N\text{-}tu)\sigma_\epsilon^2$ under all three models.

The sum of squares for interaction eliminating all other effects is equal to $SS_{\underline{\alpha\beta}} = SS_{\underline{c}} = \hat{\underline{\mu}}'W(W'S^{-1}W\ )^{-1}W'\hat{\underline{\mu}}$ and has the following expectations:

fixed effects case:

$$E(SS_{\underline{\alpha\beta}}) = tr(W'S^{-1}W)^{-1}\underline{cc}' + (t-1)(u-1)\sigma_\epsilon^2 \quad . \tag{3.2}$$

<u>mixed effects case</u> ($\underline{\alpha}_i$ <u>are fixed and</u> $\underline{\beta}_j$ <u>are random effects</u>):

$$E(SS_{\underline{\alpha\beta}}) = tr(W'S^{-1}W)^{-1}\sigma^2_{\alpha\beta} + (t-1)(u-1)\sigma^2_\epsilon \quad . \tag{3.3}$$

<u>random effects case</u>:

$$E(SS_{\underline{\alpha\beta}}) = tr(W'S^{-1}W)^{-1}\sigma^2_{\alpha\beta} + (t-1)(u-1)\sigma^2_\epsilon \quad . \tag{3.4}$$

The sum of squares for the factor involving the α_i parameters is computed as $SS_{\underline{\alpha}} = SS_{\underline{a}} = \underline{\hat{\mu}}'P(P'S^{-1}P)^{-1}P'\underline{\hat{\mu}}$ and has the following expectations:

<u>fixed effects case</u>

$$\begin{aligned} E(SS_{\underline{\alpha}}) &= tr\ P(P'S^{-1}P)^{-1}P'E(\underline{\hat{\mu}\hat{\mu}}) \\ &= tr\ P(P'S^{-1}P)^{-1}P'PE(\underline{aa}')P' + tr\ P(P'S^{-1}P)^{-1}P'S^{-1}\sigma^2_\epsilon \\ &= u^2\ tr(P'S^{-1}P)^{-1}\underline{aa}' + tr\ I_{(t-1)\times(t-1)}\sigma^2_\epsilon \\ &= u^2\ tr(P'S^{-1}P)^{-1}\underline{aa}' + (t-1)\sigma^2_\epsilon \end{aligned} \tag{3.5}$$

<u>mixed effects case</u> ($\underline{\alpha}_i$ <u>are fixed and</u> $\underline{\beta}_j$ <u>are random effects</u>):

$$\begin{aligned} E(SS_{\underline{\alpha}}) &= tr\ P(P'S^{-1}P)^{-1}E(\underline{\hat{\mu}\hat{\mu}}') \\ &= u^2\ tr(P'S^{-1}P)^{-1}\underline{aa}' + u\ tr(P'S^{-1}P)^{-1}\sigma^2_{\alpha\beta} + (t-1)\sigma^2_\epsilon \end{aligned} \tag{3.6}$$

<u>random effects case</u>:

$$E(SS_{\underline{\alpha}}) = u^2\ tr(P'S^{-1}P)^{-1}\sigma^2_\alpha + u\ tr(P'S^{-1}P)^{-1}\sigma^2_{\alpha\beta} + (t-1)\sigma^2_\epsilon \tag{3.7}$$

The sum of squares for the second factor involving the β_j parameters is computed as $SS_{\underline{b}} = SS_{\underline{\beta}} = \hat{\underline{\mu}}'Q(Q'S^{-1}Q)^{-1}Q'\hat{\underline{\mu}}$ and has the following expectations:

<u>fixed effects case</u>:

$$E(SS_{\underline{\beta}}) = t^2 \operatorname{tr}(Q'S^{-1}Q)^{-1}\underline{bb}' + (u-1)\sigma_\epsilon^2 \tag{3.8}$$

<u>mixed effects case</u> ($\underline{\alpha_i}$ <u>are fixed and</u> $\underline{\beta_j}$ <u>are random effects</u>):

$$E(SS_{\underline{\beta}}) = t^2 \operatorname{tr}(Q'S^{-1}Q)^{-1}\sigma_\beta^2 + (u-1)\sigma_\epsilon^2 \tag{3.9}$$

<u>random effects case</u>:

$$E(SS_{\underline{\beta}}) = t^2 \operatorname{tr}(Q'S^{-1}Q)^{-1}\sigma_\beta^2 + t \operatorname{tr}(Q'S^{-1}Q)^{-1}\sigma_{\alpha\beta}^2 + (u-1)\sigma_\epsilon^2 \tag{3.10}$$

In many experimental situations, single degree of freedom contrasts or subsets of degrees of freedom contrasts are desired. The expectations of these contrasts are easily described. For example, let us consider the contrast among the α_i's which is given by a_m, the contrast among the β_j's given by b_n, and the corresponding interaction of these two contrasts as given by c_{mn}. The sums of squares are computed as:

$$SS_{a_m} = \hat{\underline{\mu}}'P_m(P_m'S^{-1}P_m)^{-1}P_m'\hat{\underline{\mu}}$$

$$SS_{b_n} = \hat{\underline{\mu}}'Q_n(Q_n'S^{-1}Q_n)^{-1}Q_n'\hat{\underline{\mu}}$$

$$SS_{c_{mn}} = \hat{\underline{\mu}}'\underline{w}_{nm}(\underline{w}'_{nm}S^{-1}\underline{w}_{mn})^{-1}\underline{w}'_{mn}\hat{\underline{\mu}}$$

The expectation of these sums of squares under the various models is given below:

fixed effects case:

$$E(SS_{a_m}) = u^2(P_m' S^{-1} P_m)^{-1} a_m^2 + \sigma_\epsilon^2 \tag{3.11}$$

$$E(SS_{b_n}) = t^2(Q_n' S^{-1} Q_n)^{-1} b_n^2 + \sigma_\epsilon^2 \tag{3.12}$$

$$E(SS_{c_{mn}}) = (\underline{w}_{mn}' S^{-1} \underline{w}_{mn})^{-1} c_{mn}^2 + \sigma_\epsilon^2 \tag{3.13}$$

mixed effects case (α_i are fixed and β_j are random effects):

$$E(SS_{a_m}) = u^2(P_m' S^{-1} P_m)^{-1} a_m^2 + u(P_m' S^{-1} P_m)^{-1} \sigma_{\alpha\beta}^2 + \sigma_\epsilon^2 \tag{3.14}$$

$$\left.\begin{matrix} E(SS_{b_n}) \\ \\ E(SS_{c_{mn}}) \end{matrix}\right\} \text{ not of practical importance, but their expectations may be computed if desired.}$$

random effects case:

$$\left.\begin{matrix} E(SS_{a_m}) \\ \\ E(SS_{b_n}) \\ \\ E(SS_{c_{mn}}) \end{matrix}\right\} \text{ not of practical importance, but their expectations may be computed if desired.}$$

In order to illustrate the above formulae for the mixed effects case let us consider the following numerical example.

A 4 x 3-factorial experiment with unequal numbers of observations for four levels of temperature, A, three levels of oven, B, was conducted to ascertain the strength of the final product. The data were selected from Table 12.5 of Graybill [1961] and some observations were deleted arbitrarily.

Temp. (levels)	Oven (levels) 0		1		2	
		mean		mean		mean
0	3.3.2	2.6667	4.3	3.5000	4.6	5.0000
1	6.4	5.0000	6.2.7	5.0000	8.5.9	7.3333
2	3.4.4	3.6667	6	6.0000	5.6	5.5000
3	4.5	4.5000	3.7.9	6.3333	7.8.9	8.0000

We shall assume the model

$$y_{ijk} = \mu + \alpha_i + \beta_j + \alpha\beta_{ij} + \epsilon_{ijk}$$

where $i=0,1,2,3$; $j=0,1,2$; $k=1,2,\cdots,r_{ij}$, and α is fixed effect associated with temperature, β is random effect associated with ovens. We assume that $E\underline{\epsilon} = 0$, $E(\underline{\epsilon\epsilon}') = I\sigma^2$, $E(\underline{\beta\beta}') = I\sigma^2_\beta$, and $E(\underline{\alpha\beta}\ \underline{\alpha\beta}') = I\sigma^2_{\alpha\beta}$.

Then, using the notations defined in section 2

$$E\ \underline{y} = X(\underline{1}\ P)(\mu\ \underline{a}')'$$

$$V = Cov(\underline{y}) = XQ^*Q^{*\prime}X'\sigma^2_\beta + X(W_mW_m'+WW')X'\sigma^2_{\alpha\beta} + I\sigma^2 \quad .$$

We also assume that $\underline{y}$ is distributed normally with mean $E\ \underline{y}$ and variance-covariance V.

In this example,

$$p = \begin{bmatrix} -3 & 1 & -1 \\ -1 & -1 & 3 \\ 1 & -1 & -3 \\ 3 & 1 & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{20}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{4}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{20}} \end{bmatrix}$$

$$q = \begin{bmatrix} -1 & 1 \\ 0 & -2 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{6}} \end{bmatrix}$$

$$P = \left[\begin{bmatrix} -3 & 1 & -1 \\ -1 & -1 & 3 \\ 1 & -1 & -3 \\ 3 & 1 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \right] \begin{bmatrix} \frac{1}{\sqrt{20}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{4}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{20}} \end{bmatrix}$$

$$Q = \left[\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} -1 & 1 \\ 0 & -2 \\ 1 & 1 \end{bmatrix} \right] \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{6}} \end{bmatrix}$$

$$W = p \otimes q \; ,$$

where $\otimes$ refers to the Kronecker product, and in this example,

$$\underline{\hat{\mu}}' = (2.6667,\ 5.0000,\ 3.6667,\ 4.5000,\ 3.5000,\ 5.0000$$
$$6.0000,\ 6.3333,\ 5.0000,\ 7.3333,\ 5.5000,\ 8.0000)\ .$$

Then,

$$\underline{\hat{\mu}}'P = (4.6585,\ -1.2500,\ 3.1677)$$

$$\underline{\hat{a}}' = \tfrac{1}{3}\,\underline{\hat{\mu}}'P = (1.5528,\ -0.4133,\ 1.0559)$$

$$\underline{\hat{\mu}}'Q = (7.0711,\ 0.0000)$$

$$\underline{\hat{b}}' = \tfrac{1}{4}\,\underline{\hat{\mu}}'Q = (1.7778,\ 0.0000)$$

$$\underline{\hat{\mu}}'W = \underline{\hat{c}}' = (0.4743,\ 0.5893,\ 0.4216,\ -0.6999,\ 0.2041,\ 1.3389)\ ,$$

and

(i) $$(P'S^{-1}P)^{-1} = \begin{bmatrix} 0.7600 & 0.0707 & 0.0305 \\ 0.0707 & 0.7490 & -0.1005 \\ 0.0305 & -0.1005 & 0.6935 \end{bmatrix}$$

then

$$SS_A = 26.2185$$

and let

$$f(\underline{a}) = tr(P'S^{-1}P)^{-1}\underline{aa}'$$

(ii) $$(P_1'S^{-1}P_1)^{-1} = 0.7843$$

then

$$SS_{A_L} = 17.0207\ .$$

(iii) $(P_2'S^{-1}P_2)^{-1} = 0.7273$

then

$$SS_{A_Q} = 1.1364$$

(iv) $(P_3'S^{-1}P_3)^{-1} = 0.6780$

then

$$SS_{A_c} = 6.8032 \ .$$

(v) $$(Q'S^{-1}A)^{-1} = \begin{bmatrix} 0.6 & 0 \\ 0 & 0.5 \end{bmatrix}$$

then

$$SS_B = 30.000$$

and

$$tr(Q'S^{-1}Q)^{-1} = 1.1 \ .$$

(vi)

$$(W'S^{-1}W)^{-1} = \begin{bmatrix} 2.4238 & 0.0069 & -0.0119 & 0.0409 & 0.2305 & -0.0522 \\ 0.0069 & 2.4298 & -0.0035 & 0.2447 & 0.0670 & -0.0868 \\ -0.0119 & -0.0035 & 2.4059 & -0.0205 & -0.1153 & 0.0261 \\ 0.0409 & 0.2447 & -0.0205 & 2.4241 & 0.3962 & 0.1091 \\ 0.2305 & 0.0670 & -0.1153 & 0.3962 & 2.2319 & -0.5058 \\ -0.0522 & -0.0868 & 0.0261 & 0.1091 & -0.5058 & 1.8996 \end{bmatrix}$$

then

$$SS_{AB} = 5.5557$$

and

$$tr(W'S^{-1}W)^{-1} = 13.8151 \ .$$

Now we obtain the following analysis of variance table:

Analysis of Variance

Source of variation	d.f.	S.S.	E.M.S.
Total	29	922.0000	
CFM	1	796.6897	
Error	17	50.1687	σ^2_ϵ
A	3	26.2185	$3\ f(\underline{a}) + 2.24\ \sigma^2_{\alpha\beta} + \sigma^2_\epsilon$
A_L	1	17.0207	$\overset{7.06}{\cancel{2.36}}\ a_1^2 + \overset{2.36}{\cancel{0.78}}\ \sigma^2_{\alpha\beta} + \sigma^2_\epsilon$
A_Q	1	1.1364	$\overset{6.55}{\cancel{2.19}}\ a_2^2 + \overset{2.19}{\cancel{0.73}}\ \sigma^2_{\alpha\beta} + \sigma^2_\epsilon$
A_C	1	6.8032	$\overset{6.10}{\cancel{2.03}}\ a_3^2 + \overset{2.03}{\cancel{0.68}}\ \sigma^2_{\alpha\beta} + \sigma^2_\epsilon$
B	2	30.0000	$8.80\ \sigma^2_\beta + \sigma^2_\epsilon$
AxB	6	5.5557	$2.30\ \sigma^2_{\alpha\beta} + \sigma^2_\epsilon$

4. Construction of Main Effect Fractional Replicates and a Randomized Procedure

4.1. Introduction and notation

An s^n-factorial system is a system comprised of n factors, each at s levels. It will be assumed that s is a prime number. The space of treatment combinations, Y, is represented by the set $Y = ((i_1,i_2,\cdots,i_n) : i_k = 0,1,\cdots,$ $s-1$ for all $k=1,2,\cdots,n)$ which, clearly, contains s^n points. A standard order of the points in Y is given by the relationship between the coordinate of a point $z_v \equiv (i_1,i_2,\cdots,i_n)$, $v=0,1,\cdots,s^n-1$, and order subscript

$$v = \sum_{k=1}^{n} i_k s^{n-k} \quad . \tag{4.1.1}$$

The addition operator + between any two treatment combinations z and z' is defined as follows: If $z = (i_1,i_2,\cdots,i_n)$ and $z' = (i_1',i_2',\cdots,i_n')$ then $z + z' = (i_1'',i_2'',\cdots,i_n'')$, where $i_k'' = i_k + i_k'$ (mod s) for all $k=1,2,\cdots,n$. It follows, immediately, that the set Y is a group with respect to operator +. We denote by αz_v $(\alpha=0,1,\cdots,s-1)$, the addition of z_v itself α-times, i.e.

$$\alpha z_v = (\alpha i_1,\alpha i_2,\cdots,\alpha i_n) = (i_1',i_2',\cdots,i_n') \ , \quad (\text{mod } s) \quad .$$

Let $Y(z_v)$ be a random variable associated with the treatment combination z_v which measures the response of the system to treatment combination z_v. The relationship between the expected value of each random variable $Y(z_v)$ and treatment z_v is given by a linear function of parameters $\beta_0,\beta_1,\cdots,\beta_{s^n-1}$ as follows:

$$E[Y(z_v)] = \sum_{u=0}^{s^n-1} x_{vu}\beta_u \quad \text{for every } v=0,1,\cdots,s^n-1 \tag{4.1.2}$$

using matrix notation

$$EY(z) = X\underline{B} \quad ,$$

where

$$X = \|x_{vu}\| \;, \quad v,u=0,1,\cdots,s^n-1 \quad .$$

We shall write y_v and $\underline{y}$ as $Y(z_v)$ and $Y(z)$, respectively.

The parameter β_u have the usual interpretation of main effects and interactions of the n factors. We distinguish between linear effects, quadratic effects and effects of higher order. We also distinguish between linear-linear interactions, linear-quadratic, etc.

We further describe the structure of the s^n parameters, β_u, by considering the space B of s^n points where

$$B = ((i_1,i_2,\cdots,i_n) : i_k = 0,1,\cdots,s-1 \text{ for all } k=1,2,\cdots,n) \quad .$$

The correspondence between the parameters β_u and the points of B is given by the order relation specified by

$$u = \sum_{k=1}^{n} i_k s^{n-k} \quad .$$

We also introduce the additive operator + on the space B. The unit element of this group $\beta_0 = B(0,0,\cdots,0)$ is the mean response of all the treatment combinations. The parameter $\beta_{s^{n-k}} = B(0,0,\cdots,1,0,\cdots,0)$, $k=1,\cdots,n$, where the one is the k^{th} place, corresponds to the main effects. Referring to section 2, we may understand that this corresponds to the notation $a_k(1)$. Linear interactions correspond to points where coordinates are zero or one with at least two coordinate ones.

Let $X^{(s)}$ be the matrix whose column vectors are the coefficients of orthogonal polynomials of order s, namely

$$X^{(s)} = \begin{bmatrix} 1 & \gamma_{01} & \cdots & \gamma_{0,s-1} \\ 1 & \gamma_{11} & \cdots & \gamma_{1,s-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \gamma_{s-1,1} & \cdots & \gamma_{s-1,s-1} \end{bmatrix}, \qquad (4.1.3)$$

For example,

$$X^{(2)} = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \quad \text{and} \quad X^{(3)} = \begin{bmatrix} 1 & -1 & 1 \\ 1 & 0 & -2 \\ 1 & 1 & 1 \end{bmatrix} .$$

The inner product of any two different column vectors of $X^{(s)}$ is zero. The matrix $X^{(s^n)}$ can be defined recursively for all $n \geq 2$ by

$$X^{(s^n)} = \begin{bmatrix} X^{(s^{n-1})} & \gamma_{01}X^{(s^{n-1})} & \cdots & \gamma_{0,s-1}X^{(s^{n-1})} \\ X^{(s^{n-1})} & \gamma_{11}X^{(s^{n-1})} & \cdots & \gamma_{1,s-1}X^{(s^{n-1})} \\ \vdots & \vdots & \ddots & \vdots \\ X^{(s^{n-1})} & \gamma_{s-1,1}X^{(s^{n-1})} & \cdots & \gamma_{s-1,s-1}X^{(s^{n-1})} \end{bmatrix} \qquad (4.1.4)$$

In other words, the matrix $X^{(s^n)}$ is obtained from $X^{(s^{n-1})}$ by Kronecker multiplication of $X^{(s^{n-1})}$ by $X^{(s)}$ from the left, i.e., $X^{(s^n)} = X^{(s)} \otimes X^{(s^{n-1})}$. The coefficient matrix X in (4.1.2) is $X^{(s^n)}$.

Writing X as $X^{(s^n)}$, the observational equation for any factorial treatment design may be represented as:

$$\underline{y} = X\underline{B} + \epsilon \quad , \qquad (4.1.5)$$

where it is assumed that $E(\epsilon\epsilon') = I\sigma^2$, where I is the N×N identity matrix, and where $\underline{B}$ is the vector of individual treatment contrasts.

Consider the following expression:

$$\underline{y} = [X_1 \quad X_2] \begin{bmatrix} \underline{B}_p \\ \underline{B}_{N-p} \end{bmatrix} + \underline{\epsilon} \quad , \qquad (4.1.6)$$

where $\underline{B}_p$ is a given parameter vector, $p \le N$, X_1 is an N×p matrix, and X_2 is an N×(N-p) matrix. Since $r(X) = N$ and $r(X_1) = p$, then there exists at least one nonsingular p×p matrix X_{11} in X_1.

After rearranging the row orders in $\underline{y}$, $[X_1 \;\; X_2]$, and $\underline{\epsilon}$ respectively, we obtain the following matrix equation:

$$\begin{bmatrix} \underline{y}_p \\ \underline{y}_{N-p} \end{bmatrix} = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \begin{bmatrix} \underline{B}_p \\ \underline{B}_{N-p} \end{bmatrix} + \begin{bmatrix} \underline{\epsilon}_p \\ \underline{\epsilon}_{N-p} \end{bmatrix} , \qquad (4.1.7)$$

where X_{11} is a nonsingular p×p matrix. Then

$$\underline{y}_p = [X_{11} \;\; X_{12}] \begin{bmatrix} \underline{B}_p \\ \underline{B}_{N-p} \end{bmatrix} + \underline{\epsilon}_p \qquad (4.1.8)$$

and the observations in $\underline{y}_p$ yield a saturated fractional replicate for the given parameters in $\underline{B}_p$ (see Banerjee and Federer [1963], [1964], [1966], [1968], [1968].) .

4.2. Construction of any specified fractional replicate

In a talk given at the 1967 Spring Statistical Meetings in Atlanta, Georgia (Paik and Federer [1967b]), a procedure was given for constructing any specified fractional replicate from any factorial treatment design. The following common steps for constructing any fractional replicate as given by Paik and Federer [1967b] are described below. These authors discuss the construction problem in detail and they present a number of short cuts amply illustrated with examples.

Step 1. Given the design matrix and parameter and observation vectors $X\underline{B} = E(\underline{y})$ in any fashion, we now rearrange the parameter matrix such that the p parameters, $p < N$, are arranged to have the p parameters of interest first and N-p parameters not of interest last to obtain $\underline{B}$ rearranged $(\underline{B}^{*\prime}_{p}\underline{B}^{*}_{N-p})$. This also rearranges the columns of X to produce another matrix denoted as X^{*} such that

$$X^{*}\underline{B}^{*} = E(\underline{y})$$

$$\left(\underset{N\times p}{X_1^{*}} \quad \underset{N\times(N-p)}{X_2^{*}}\right)\begin{bmatrix} \underline{B}^{*}_{p} \\ \\ \underline{B}^{*}_{N-p} \end{bmatrix} = E(\underline{y}) \quad .$$

Step 2. Search through rows of X_1^{*} until there is an X_{11}, $p\times p$, which is nonsingular.

Step 3. Corresponding to the rows in X_{11} will be rows in X_1^{*} and observations in Y for the designated treatments. Rearrange the observations in Y into $[Y_p^{*\prime} \quad Y_{N-p}^{*\prime}]'$ corresponding to the rows in X_{11} from X_1^{*}. The observations in Y_p yield a saturated design for the parameters in $\underline{B}^{*}_{p}$. This obtained set is one of the possible sets. All possible sets are found by defining all X_{11} which have an invers.

4.3. An invariant property of $|X_{11}' \quad X_{11}|$

In a 2^n-factorial, the matrix $X^{(2)}$ corresponding to the observation vector for treatments $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ is $\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$ and $X_{\alpha}^{(2)}$ corresponding to

$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} + \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, (mod 2), is $\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$, then the relationship between $X_\alpha^{(2)}$ and $X^{(2)}$ is as follows:

$$X_\alpha^{(2)} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} X^{(2)}, \text{ or } \quad X_\alpha^{(2)} = X^{(2)} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} .$$

Also, $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = I_{2\times 2}$ and $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = I_{2\times 2}$.

In a 3^n-factorial, the matrix $X^{(3)}$ corresponding to $\begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix}$ is $\begin{pmatrix} 1 & -1 & 1 \\ 1 & 0 & -2 \\ 1 & 1 & 1 \end{pmatrix}$ and $X_\alpha^{(3)}$ corresponding to $\begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix} + \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$, (mod 3), in $\begin{pmatrix} 1 & 0 & -2 \\ 1 & 1 & 1 \\ 1 & -1 & 1 \end{pmatrix}$ and $X_\beta^{(3)}$ corresponding to $\begin{pmatrix} 2 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix} + \begin{pmatrix} 2 \\ 2 \\ 2 \end{pmatrix}$, (mod 3), is $\begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 0 & -2 \end{pmatrix}$.

Let $A = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$, $B = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1/2 & -1/2 \\ 0 & 3/2 & -1/2 \end{pmatrix}$ and let $C = \begin{pmatrix} -1/2 & -1/2 \\ 3/2 & -1/2 \end{pmatrix}$, then the relationships among $X_\alpha^{(3)}$, $X_\beta^{(3)}$ and $X^{(3)}$ are as follows:

$$X_\alpha^{(3)} = AX^{(3)} \quad \text{or} \quad X_\alpha^{(3)} = X^{(3)}B$$

$$X_\beta^{(3)} = A^2X^{(3)} \quad \text{or} \quad X_\beta^{(3)} = X^{(3)}B^2 \quad .$$

In this case, we can easily see that $A^3 = I_{3\times 3}$, $B^3 = I_{3\times 3}$, $|A|$ = unity, $|B|$ = unity and also $C^3 = I_{2\times 2}$ and $|C|$ = unity.

<u>Lemma 4.1.</u> In an s^n-factorial (s is a prime number), if the $X^{(s)}$ is the corresponding matrix to $(0,1,\cdots,s-1)'$ and $X_1^{(s)}$ is the corresponding matrix to $(1,2,\cdots,s-1,0)' = (0,1,\cdots,s-1)' + (1,1,\cdots,1)'$, (mod s), and $X_i^{(s)}$ is the matrix corresponding to $(i,i+1,\cdots,s-1,0,\cdots,i-1) = (0,1,\cdots,s-1) + (i,i,\cdots,i)$, (mod s), then

(i) there exist $s\times s$ matrices A and B such that

$$X_1^{(s)} = AX^{(s)} , \qquad X_i^{(s)} = A^i X^{(s)} ,$$

$$X_1^{(s)} = X^{(s)}B , \quad \text{and} \quad X_i^{(i)} = X^{(s)}B^i ,$$

(ii) $A^s = I_{s\times s}$ and $B^s = I_{s\times s}$ so $|A| = 1$ and $|B| = 1$,

(iii) the matrix B has a form

$$\begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & C & \\ 0 & & & \end{bmatrix}$$

and $C^s = I_{(s-1)\times(s-1)}$ and $|C| = 1$.

(iv) $\sum_{i=0}^{s-1} C^i = 0$.

(The proof is omitted because of time requirements.)

Let $Y_p(s^n)$ be a saturated main effect plan, write this as Y_p, represented by the treatment combinations such as given by a $p \times n$ matrix in an s^n-factorial and let X_{11} be a $p \times p$ coefficient matrix of the main effect parameters corresponding to the plan Y_p.

Let $J(i_1, i_2, \cdots, i_n)$ be a $p \times n$ matrix such that

$$J(i_1, i_2, \cdots, i_n) = \begin{bmatrix} i_1 & i_2 & \cdots & i_n \\ i_1 & i_2 & \cdots & i_n \\ \vdots & \vdots & \ddots & \vdots \\ i_1 & i_2 & \cdots & i_n \end{bmatrix}$$

where $i_k = 0, 1, \cdots, s-1$ for all $k = 1, 2, \cdots, n$, and $X_{11,v}$ be a $p \times p$ coefficient matrix of the main effect parameters corresponding to the plan $Y_{p,v} = Y_p + J(i_1, i_2, \cdots, i_n)$, (mod s), then we obtain the following theorem.

<u>Theorem 4.1.</u> If Y_p is a saturated main effect plan, then $Y_{p,v}$ also is a saturated main effect plan and $|X'_{11,v} X_{11,v}| = |X'_{11} X_{11}|$.

(No proof is given because of time limitations.)

The meaning of this theorem is that if Y_p is not a subgroup (in the algebraic sense), or a regular fraction, of a complete s^n-factorial, given a main effect plan Y_p, $Y_p + J(i_1, i_2, \cdots, i_n)$, $i_k = 0, 1, \cdots, s-1$ for all $k = 1, \cdots, n$, may produce s^n different main effect plans, but determinants of their information matrices have the same value.

A main effect plan $Y_{p,u}$ in an s^n-factorial is said to be <u>independent</u> of a main effect plan Y_p if $Y_{p,u}$ cannot be constructed by the procedure

$Y_p + J(i_1, i_2, \cdots, i_n)$, $i_k = 0, 1, \cdots, s-1$ for all $k = 1, 2, \cdots, n$. If $Y_{p,u}$ and Y_p are not independent then the set of $\{Y_p + J(i_1, i_2, \cdots, i_n)\}$ is generated by Y_p. Using this criterion, we may list every independent main effect plan given an s^n-factorial. We present a complete list in the cases for 2^2, 2^3, and 2^4-factorials in the Appendix.

4.4. Optimality of the saturated main effect plan

If we find a fraction which has a maximum value of $|X_{11}|$ or of $|X_{11}' X_{11}|$ among all saturated plans, then it will be an optimum fractional replicate in the sense utilized by a number of authors (e.g., Hoel [1958], Kiefer and Wolfowitz [1959,1959,1960], Banerjee and Federer [1963,1966], Karlin and Studden [1966], etc.).

Referring to the paper by Paik and Federer [1967b] and section 4.2 and 4.3, we may find the following generators of the optimum main effect plan in a 2^4-factorial and in a 3^3-factorial.

(i) Saturated main effect plan in a 2^n-factorial.

In this case, every $|X_{11}' X_{11}|$ has one of the four values, i.e., $2304 = 9(2^{10})/4$, $1024 = 2^{10}$, $256 = 2^8$, or zero. The set of optimum designs is a set generated by

0000
0111
1011
1101
1110

(ii) Saturated main effect plan in a 3^3-factorial.

In this case, every $|X_{11}' X_{11}|$ has one of the five values, i.e.,

$746496 = 3^5(2^{10})$, $419904 = 3^8(2^5)$, $186624 = 2^8(3^6)$, $46656 = 3^6(2^6)$, or zero.

The sets of optimum designs are the sets generated by

(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)
000	000	000	000	000	000	000	000	000
021	012	012	011	011	012	011	022	022
101	102	021	101	102	101	101	202	202
112	110	102	112	110	110	110	220	220
120	121	110	120	201	211	122	211	011
202	201	211	210	121	021	212	121	101
210	220	220	222	222	222	221	112	110

4.5. A randomized procedure for saturated main effect fractional replications

From Banerjee and Federer [1964], the least-squares estimator $X_{11}^{-1}\,\underline{y}$ of $\underline{B}^* = \underline{B}_p + X_{11}^{-1} X_{12} B_{N-p}$ is a best linear unbiased estimator of $\underline{B}_p^*$. But if the objective is to estimate $\underline{B}_p$ there exists no fractional replicate design and least-squares estimator which yields best linear unbiased estimators of $\underline{B}_p$. Ehrenfeld and Zacks [1961] presented the randomized procedures for the regular fractional replicates, and Zacks [1963,1964] showed that unbiased estimator of $\underline{B}_p$ in the saturated fractional replicate case exists only if one randomizes over-all designs of a certain structure for the case of 2^n system.

A similar method to the Randomized Procedure I in their papers is given for saturated non-orthogonal main effect fractional replicates and an unbiased estimator of the main effect vector is presented below. However, the explicit expression of the variance of the estimator is still a problem.

Suppose a plan Y_p was chosen at random from a set $\{Y^*_{p,v}$; $v=0,1,\cdots,N-1$, where $N=s^n\}$ generated by a saturated main effect fractional replicate Y^*_p and sets $\{X_{11,v}$; $v=0,1,\cdots,N-1\}$ and $\{X_{12,v}$; $v=0,1,\cdots\}$ are the sets of pxp coefficient matrix of the main effect parameters and of px(N-p) coefficient matrix of the nuisance parameters

$\{Y^*_{p,v}\ ;\ v=0,1,\cdots,N-1\}$, respectively. Let $\underline{B}^*_p = X_{11}^{-1}\, Y_p(z)$ be the conditional least-squares estimator of $\underline{B}_p$ under plan Y_p, where $Y_p(z)$ is the observation vector and X_{11} be a p×p coefficient matrix corresponding to the main effect parameter under the plan Y_p in an s^n-factorial and let X^* be an N×N coefficient matrix of the parameter vector $[\underline{B}_p'\ \underline{B}_{N-p}']'$ in an s^n-factorial.

Suppose that X^* is partitioned as

$$X^* = [X_1 \quad X_2] = \begin{bmatrix} X_{11} & X_{12} \\ & \\ X_{21} & X_{22} \end{bmatrix}, \tag{4.5.1}$$

then, since $X^{*\prime}X^*$ is a diagonal matrix, it is easy to verify that

$$E_v X_{11,v}' X_{11,v} = \frac{1}{p}\, X_1' X_1 \tag{4.5.2}$$

and

$$E\, X_{11}^{-1} X_{12} = 0 \quad . \tag{4.5.4}$$

(The proof is not presented owing to time limitations.)

<u>Theorem 4.2</u>. Suppose a saturated main effect plan Y_p is chosen at random from a set generated by a plan Y^*_p, then the least square estimator $\hat{\underline{B}}^* = X_{11}^{-1} Y_p(z)$ of $\underline{B}^*_p = \underline{B}_p + X_{11}^{-1} X_{12} \underline{B}_{N-p}$ given X_{11} is an unbiased estimator of $\underline{B}_p$.

(The proof is not presented owing to time limitations.)

5. Expectation of Mean Squares for Fractional Replicates

In the event that some of the subclass numbers are zero, a fractional replicate results. Since missing subclasses involves additional considerations, this topic is discussed in a separate section from the case when the subclasses are not missing. Using the following notation as defined previously

$$\underline{y} = X\underline{\mu}_v + \epsilon$$

$\underline{y}$ is an $N\times 1$ vector

$\underline{\mu}_v$ is a $v\times 1$ vector , $v \le tu$

$$\underline{\alpha} = p^*\underline{a}^*$$

$$\underline{\beta} = q^*\underline{b}^*$$

$$\alpha\beta = W^*\underline{c}^* \quad , \quad W^* = p^* \otimes q^*$$

we now set up the expected values of sums of squares. Let P_v^*, Q_v^*, and W_v^* be the $v\times t$, $v\times u$, and $v\times tu$ matrices, respectively, and satisfy the following equation

$$\underline{\mu}_v = \mu\underline{1}_v + P_v^*\underline{a}^* + Q_v^*\underline{b}^* + W_v^*\underline{c}^*$$

Let

$$W_v^* = [W_{11} \quad W_{12}] ,$$

where W_{11} is a $v\times v$ non-singular matrix and W_{12} is a $v\times(tu-v)$ matrix, and let

$$W_{11} = \begin{bmatrix} \frac{1}{\sqrt{ut}} \mathbf{1} & W_P & W_Q & W_c \end{bmatrix} \text{ such that}$$

$$W_P = \frac{1}{\sqrt{u}} P_v$$

$$W_Q = \frac{1}{\sqrt{t}} Q_v$$

where P_v, Q_v are submatrices of P_v, Q_v are submatrices of P_v^* and Q_v^* such that

$$P_v^* = \begin{bmatrix} \frac{1}{\sqrt{t}} \underline{\mathbf{1}} & \underline{P}_v \end{bmatrix}$$

$$Q_v^* = \begin{bmatrix} \frac{1}{\sqrt{u}} \underline{\mathbf{1}} & \underline{Q}_v \end{bmatrix}$$

Now, let

$$Z = W_{11}^{-1}$$

and let

$$Z = \begin{bmatrix} Z_1 \\ Z_P \\ Z_Q \\ Z_W \end{bmatrix} = \begin{bmatrix} Z_1 \\ Z_{P1} \\ \vdots \\ Z_{P,t-1} \\ Z_{Q1} \\ \vdots \\ Z_{Q,u-1} \\ Z_{W1} \\ \vdots \\ Z_{W1(t-1)(u-1)} \end{bmatrix}$$

where Z_P, Z_Q, and Z_W are $(t-1)\times v$, $(u-1)\times v$, and $(t-1)(u-1)\times v$ matrices, respectively, and $Z_1, Z_{P1}, \cdots, Z_{W,(t-1)(u-1)}$ are $1\times v$ row vectors, then $Z_P P_v = \sqrt{u}\ I$, $Z_Q Q_v = \sqrt{t}\ I$ and $Z_W W_v = I$.

Now, we obtain

$$Z_P\ \underline{\mu}_v = \sqrt{u}\ I\underline{a} + I\underline{c}_{m.} + Z_P W_{12} \underline{c}_{W_{12}}$$

$$Z_{Pm}\ \underline{\mu}_v = \sqrt{u}\ a_m + c_{m0} + Z_{Pm} W_{12} \underline{c}_{W_{12}}$$

$$Z_Q\ \underline{\mu}_v = \sqrt{t}\ I\underline{b} + I\underline{c}_{\cdot n} + Z_Q W_{12} \underline{c}_{W_{12}}$$

$$Z_W\ \underline{\mu}_v = I\underline{c}_{Wc} + Z_W W_{12} \underline{c}_{W_{12}}$$

where

$$c^{*\prime} = (c_{00}, \underline{c}'_{m.}, \underline{c}'_{\cdot n}, \underline{c}'_{W0}, \underline{c}'_{W_{12}}) \quad .$$

The sums of squares for each effect is obtained as follows:

$$SS_{\underline{a}} = \hat{\underline{\mu}}'_v\ Z'_P (Z_P\ S^{-1}\ Z'_P)^{-1}\ Z_P \hat{\underline{\mu}}_v$$

$$SS_{an} = \hat{\underline{\mu}}'_v\ Z'_{Pm} (Z'_{Pm}\ S^{-1}\ Z'_{Pm})^{-1}\ Z_{Pm} \hat{\underline{\mu}}_v$$

$$SS_{\underline{b}} = \hat{\underline{\mu}}'_v\ Z'_Q (Z_Q\ S^{-1}\ Z'_Q)^{-1}\ Z_Q \hat{\underline{\mu}}_v$$

$$SS_{\underline{c}} = \hat{\underline{\mu}}'_v\ Z'_W (Z_W\ S^{-1}\ Z'_W)^{-1}\ Z_W \hat{\underline{\mu}}_v$$

where

$$S^{-1} = (X'X)^{-1} \quad .$$

The expected value of sums of squares SS_α for a two-factor experiment is:

α, β are both fixed effects

$$E(SS_{\underline{\alpha}}) = u\ tr(Z_pS^{-1}Z_p')^{-1}\underline{aa}' + \sqrt{u}\ tr(Z_pS^{-1}Z_p')^{-1}(Z_pW_{12}\underline{c}_{W_{12}}\underline{a}'+\underline{ac}_{W_{12}}'W_{12}'Z_p')$$

$$+ tr(Z_pS^{-1}Z_p')^{-1}Z_pW_{12}\underline{c}_{W_{12}}\underline{c}_{W_{12}}'W_{12}'Z_p' + (t-1)\sigma^2$$

$$= u\ tr(Z_pS^{-1}Z_p')^{-1}\underline{aa}' + (t-1)\sigma^2 \quad \text{if} \quad \underline{c}_{W_{12}} = 0 .$$

β is random effect, α is a fixed effect

$$E(SS_{\underline{\alpha}}) = u\ tr(Z_pS^{-1}Z_p')^{-1}\underline{aa}' + tr[(Z_pS^{-1}Z_p')^{-1}+Z_pW_{12}(Z_pS^{-1}Z_p')^{-1}W_{12}'Z_p']\sigma^2_{\alpha\beta}$$

$$+ (t-1)\sigma^2$$

$$= u\ tr(Z_pS^{-1}Z_p')\underline{aa}' + tr(Z_pS^{-1}Z_p')^{-1}\sigma^2_{\alpha\beta} + (t-1)\sigma^2 \quad \text{if} \quad \underline{c}_{W_{12}} = 0 .$$

α, β are both random effects

$$E(SS_{\underline{\alpha}}) = u\ tr(Z_pS^{-1}Z_p')^{-1}\sigma^2_\alpha + tr[(Z_pS^{-1}Z_p')^{-1}+Z_pW_{12}(Z_pS^{-1}Z_p')^{-1}W_{12}'Z_p']\sigma^2_{\alpha\beta}$$

$$+ (t-1)\sigma^2$$

$$= u\ tr(Z_pS^{-1}Z_p')^{-1}\sigma^2_\alpha + tr(Z_pS^{-1}Z_p')^{-1}\sigma^2_{\alpha\beta} + (t-1)\sigma^2 \quad \text{if} \quad \underline{c}_{W_{12}} = 0 .$$

If $\underline{c}_{W_{12}} = 0$, this is equivalent to setting each of the parameters in $\underline{B}_{N-p}$ equal to zero.

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APPENDIX

Classifications of the Saturated Main Effect Plans in 2^2, 2^3, and 2^4-factorials

1. Generator of the saturated main effect plans in a 2^2-factorial.

   There is only one generator and $|X_{11}'X_{11}| = 16$

$$
\begin{array}{c} 00 \\ 01 \\ 10 \end{array}
\left\{
\begin{bmatrix} 00 \\ 01 \\ 10 \end{bmatrix} + \begin{bmatrix} 00 \\ 00 \\ 00 \end{bmatrix} = \begin{bmatrix} 00 \\ 01 \\ 10 \end{bmatrix},
\begin{bmatrix} 00 \\ 01 \\ 10 \end{bmatrix} + \begin{bmatrix} 01 \\ 01 \\ 01 \end{bmatrix} = \begin{bmatrix} 01 \\ 00 \\ 11 \end{bmatrix},
\begin{bmatrix} 00 \\ 01 \\ 10 \end{bmatrix} + \begin{bmatrix} 10 \\ 10 \\ 10 \end{bmatrix} = \begin{bmatrix} 10 \\ 11 \\ 00 \end{bmatrix},
\begin{bmatrix} 00 \\ 01 \\ 10 \end{bmatrix} + \begin{bmatrix} 11 \\ 11 \\ 11 \end{bmatrix} = \begin{bmatrix} 11 \\ 10 \\ 01 \end{bmatrix}
\right\}
$$

2. Generators of the saturated main effect plans in a 2^3-factorial.

   (i) $|X_{11}'X_{11}| = 256 = 2^8$.

000*
011
101
110

   (ii) $|X_{11}'X_{11}| = 64 = 2^6$.

000	000	000	000	000	000	000
100	100	100	001	101	011	011
101	101	110	101	110	101	110
110	111	111	111	111	111	111

   (iii) $|X_{11}'X_{11}| = 0$

000*	000*	000*	000*	000*	000*
001	001	010	001	010	011
010	100	100	110	101	100
011	101	110	111	111	111

* A regular fraction of a 2^3-factorial. (This yields only two plans instead of $2^3 = 8$ plans.)

3. Generators of the saturated main effect plans in a 2^4-factorial.

(i) $|X'_{11}X_{11}| = 2304 = 3^2(2^8)$

0000
0111
1011
1101
1110

(ii) $|X'_{11}X_{11}| = 1024 = 2^{10}$

0000	0000	0000	0000	0000	0000	0000	0000
0011	0011	0101	0110	0011	0011	0101	0110
0101	1001	1001	1010	0101	1001	1001	1010
0110	1010	1100	1100	0110	1010	1100	1100
1000	0100	0010	0001	1001	0101	0011	0011

0000	0000	0000	0000	0000	0000	0000	0000
0011	0011	0101	0110	0011	0011	0101	0110
0101	1001	1001	1010	0101	1001	1001	1010
1110	1110	1110	1101	1110	1110	1110	1101
1000	0100	0010	0001	1011	0111	0111	0111

0000	0000	0000	0000
0011	0011	0101	0110
0101	1001	1001	1010
1110	1110	1110	1101
1101	1101	1011	1011

(iii) $|X'_{11}X_{11}| = 256 = 2^8$

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0001	0001	0001	0010
0011	0011	0101	0110	0011	0011	0101	0110
0101	1001	1001	1010	0111	1011	1101	1110
1000	0100	0010	0001	1000	0100	0010	0001

0000	0000	0000	0000	0000	0000	0000	0000
0011	0011	0101	0110	0001	0001	0001	0010
0101	1001	1001	1010	0011	0011	0101	0110
0111	1011	1101	1110	0101	1001	1001	1010
1000	0100	0010	0001	1001	0101	0011	0011

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0011	0011	0101	0110
0011	0011	0101	0110	0101	1001	1001	1010
0111	1011	1101	1110	0111	1011	1101	1110
1001	0101	0011	0011	1001	0101	0011	0011

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0001	0001	0001	0010
0011	0011	0101	0110	0011	0011	0101	0110
0101	1001	1001	1010	0111	1011	1101	1110
1010	0110	0110	0101	1010	0110	0110	0101

0000	0000	0000	0000	0000	0000	0000	0000
0011	0011	0101	0110	0001	0001	0001	0010
0101	1001	1001	1010	0011	0011	0101	0110
0111	1011	1101	1110	0101	1001	1001	1010
1010	0110	0110	0101	1100	1100	1010	1001

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0011	0011	0101	0110
0011	0011	0101	0110	0101	1001	1001	1010
0111	1011	1101	1110	0111	1011	1101	1110
1100	1100	1010	1001	1100	1100	1010	1001

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0001	0001	0001	0010
0011	0011	0101	0110	0011	0011	0101	0110
0101	1001	1001	1010	0111	1011	1101	1110
1011	0111	0111	0111	1011	0111	0111	0111

0000	0000	0000	0000	0000	0000	0000	0000
0011	0011	0101	0110	0001	0001	0001	0010
0101	1001	1001	1010	0011	0011	0101	0110
0111	1011	1101	1110	0101	1001	1001	1010
1011	0111	0111	0111	1101	1101	1011	1011

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0011	0011	0101	0110
0011	0011	0101	0110	0101	1001	1001	1010
0111	1011	1101	1110	0111	1011	1101	1110
1101	1101	1011	1011	1101	1101	1011	1011

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0001	0001	0001	0010
0011	0011	0101	0110	0011	0011	0101	0110
0101	1001	1001	1010	0111	1011	1101	1110
1110	1110	1110	1101	1110	1110	1110	1101

0000	0000	0000	0000	0000	0000	0000	0000
0011	0011	0101	0110	0001	0001	0001	0010
0101	1001	1001	1010	0011	0011	0101	0110
0111	1011	1101	1110	0101	1001	1001	1010
1110	1110	1110	1101	1111	1111	1111	1111

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0011	0011	0101	0110
0011	0011	0101	0110	0101	1001	1001	1010
0111	1011	1101	1110	0111	1011	1101	1110
1111	1111	1111	1111	1111	1111	1111	1111

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0001	0001	0001	0010
0011	0011	0101	0110	0011	0011	0101	0110
1101	1101	1011	1011	1111	1111	1111	1111
1000	0100	0010	0001	1000	0100	0010	0001

0000	0000	0000	0000	0000	0000	0000	0000
0011	0011	0101	0110	0001	0001	0001	0010
0101	1001	1001	1010	0011	0011	0101	0110
1111	1111	1111	1111	1101	1101	1011	1011
1000	0100	0010	0001	1001	0101	0011	0011

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0011	0011	0101	0110
0011	0011	0101	0110	0101	1001	1001	1010
1111	1111	1111	1111	1110	1110	1110	1101
1001	0101	0011	0011	1010	0110	0110	0101

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0001	0001	0001	0010
0011	0011	0101	0110	0011	0011	0101	0110
1101	1101	1011	1011	1111	1111	1111	1111
1010	0110	0110	0101	1010	0110	0110	0101

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0011	0011	0101	0110
0110	1010	1100	1100	0101	1001	1001	1010
1111	1111	1111	1111	1110	1110	1110	1101
1010	0110	0110	0101	1100	1100	1010	1001

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0001	0001	0001	0010
0110	1010	1100	1100	0011	0011	0101	0110
1111	1111	1111	1111	1010	0110	0110	0101
1100	1100	1010	1001	1100	1100	1010	1001

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0001	0001	0001	0010
0011	0011	0101	0110	0011	0011	0101	0110
1101	1101	1011	1011	1111	1111	1111	1111
1011	0111	0111	0111	1011	0111	0111	0111

0000	0000	0000	0000	0000	0000	0000	0000
0011	0011	0101	0110	0001	0001	0001	0010
0101	1001	1001	1010	0110	1010	1100	1100
1111	1111	1111	1111	1111	1111	1111	1111
1011	0111	0111	0111	1011	0111	0111	0111

0000	0000	0000	0000	0000	0000	0000	0000
0011	0011	0101	0110	0001	0001	0001	0010
0101	1001	1001	1010	0011	0011	0101	0110
1111	1111	1111	1111	1010	0110	0110	0101
1101	1101	1011	1011	1101	1101	1011	1011

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0011	0011	0101	0110
0110	1010	1100	1100	0101	1001	1001	1010
1111	1111	1111	1111	1111	1111	1111	1111
1101	1101	1011	1011	1110	1110	1110	1101

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0011	0011	0101	0110
0011	0011	0101	0110	0101	1001	1001	1010
1010	0110	0110	0101	1110	1110	1110	1101
1110	1110	1110	1101	1111	1111	1111	1111

0000	0000	0000	0000
0001	0001	0001	0010
0011	0011	0101	0110
1010	0110	0110	0101
1111	1111	1111	1111

(iv) $|X'_{11}X_{11}| = 0$

0000	0000	0000	0000	0000	0000	0000	0000
0011	0011	0101	0110	0011	0011	0101	0110
0101	1001	1001	1010	0101	1001	1001	1010
0110	1010	1100	1100	0111	1011	1101	1110
0001	0001	0001	0010	0001	0001	0001	0010

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0011	0011	0101	0110
0011	0011	0101	0110	0101	1001	1001	1010
0101	1001	1001	1010	0111	1011	1101	1110
0010	0010	0100	0100	0010	0010	0100	0100

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0001	0001	0001	0010
0110	1010	1100	1100	0011	0011	0101	0110
0111	1011	1101	1110	0101	1001	1001	1010
0010	0010	0100	0100	0100	1000	1000	1000

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0001	0001	0001	0010
0011	0011	0101	0110	0110	1010	1100	1100
0111	1011	1101	1110	0111	1011	1101	1110
0100	1000	1000	1000	1000	0100	0010	0001

0000	0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0001	0001	0001	0010
0110	1010	1100	1100	0110	1010	1100	1100
0111	1011	1101	1110	1111	1111	1111	1111
1010	0110	0110	0101	1001	0101	0011	0011

0000	0000	0000	0000	0000	0000	0000	0000
0011	0011	0101	0110	0011	0011	0101	0110
0101	1001	1001	1010	0101	1001	1001	1010
1111	1111	1111	1111	1111	1111	1111	1111
1010	0110	0110	0101	1100	1100	1010	1001

0000	0000	0000	0000	0000	0000	0000
0001	0001	0001	0010	0001	0001	0010
0110	1010	1100	1100	0011	0101	0110
1111	1111	1111	1111	0010	0100	0100
1110	1110	1110	1101	1100	1010	1001

0000	0000	0000	0000	0000	0000
0001	0001	0001	0001	0001	0010
0110	1010	1100	0011	0101	0110
1111	1111	1111	1101	1011	1011
1000	0100	0010	1100	1010	1001

0000	0000	0000
0001	0001	0010
0011	0101	0110
1111	1111	1111
1100	1010	1001